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Fundamental Physics and Model Assumptions in Turbulent Combustion Models for Aerospace Propulsion

Venkateswaran Sankaran*
Air Force Research Lab, Edwards AFB, CA 93524, USA

Charles L. Merkle†
Purdue University, West Lafayette, IN 47906, USA

The paper provides a fundamental overview of turbulence and turbulent combustion models for large eddy simulations of reacting flowfields. The focus is on examining model assumptions in the context of aerospace propulsion applications, which typically involve high-speed flows, high pressures, compressible phenomena such as shocks, ignition dynamics and acoustic instabilities. Models considered include the dynamic Smagorinsky model for turbulence, and laminar flamelets, transported-PDF and the linear eddy model (LEM) for turbulent combustion. Validation procedures are devised to determine modeling gaps and identify areas where model enhancements are needed.

I. Introduction

Turbulent combustion modeling has seen significant developments in recent decades. This progress has been enabled by a number of factors such as the emergence of highly scalable computational architectures, high-frequency laser-based diagnostics for validation data, advanced numerical techniques and new classes of turbulence, combustion and turbulent combustion models. These developments are, in turn, addressing the growing need for high-fidelity time-accurate solutions of complex reacting flows in the fields of combustion, energy conversion and propulsion. In this article, we review some of the fundamental turbulence and turbulent combustion models[1–6] and provide assessments of the underlying assumptions and their applicability to problems of relevance to aerospace propulsion, namely, rockets, gas turbines, augmentors and scramjet engines. The overall objectives are to shed light on the strengths and limitations of the current state-of-the-art and to develop approaches to make further progress.

A key theme of the current study is the examination of fundamental model assumptions for conditions relevant to aerospace propulsion applications. This typically means the presence of high-speed flows, high pressures, compressible phenomena such as shocks, ignition dynamics, and acoustics coupling, which are aspects that are frequently ignored in fundamental turbulent combustion studies. Moreover, our focus is on so-called off-design operation of propulsion devices. In other words, we are particularly interested in phenomena such as combustion instability and ignition (and extinction), which are highly dynamic and therefore difficult to predict. For example, Fig. 1(a) shows the ignition of mono-methyl hydrazine (MMH) and red fuming nitric acid (RFNA) injected into a container that is initially filled with Argon.[7] For the gas-phase results shown, the dynamics of ignition depend upon the interaction between the chemical kinetics and the turbulence dynamics of the propellant streams. For liquid propellants, the situation is further complicated by the presence of multi-phase effects such as atomization and vaporization; however, we restrict the current study to gas-phase phenomena to keep the problem reasonably tractable. Figure 1(b) shows an example of an unstable gas-gas rocket combustor. Here, methane fuel mixes with decomposed peroxide as the oxidizer. Combustion instabilities occur when the acoustic modes in the chamber couple with the

*Senior Scientist, Aerospace Systems Directorate, Senior Member.
†Emeritus Professor, Dept of Mechanical Engineering, Senior Member.

combustion dynamics, leading to a highly unstable flame. In the example shown, the dynamics in the oxidizer post lead to an interruption in the propellant flow, which in turn causes a pulsatile flame that is in synchronization with the pressure oscillations in the combustion chamber.[8] The combustion zone is very dynamic and is characterized by multiple extinction and re-ignition events. Again, the coupling between the combustion and the acoustics modes is influenced by a number of factors including chemical kinetics and turbulence dynamics. Finally, in the case of scramjet problems, the turbulence and combustion are further influenced by the presence of shocks. Accurate prediction of such physical phenomena depends intimately on the modeling of the fine-scale dynamics of turbulence and chemistry, a problem that is collectively referred to as turbulent combustion.

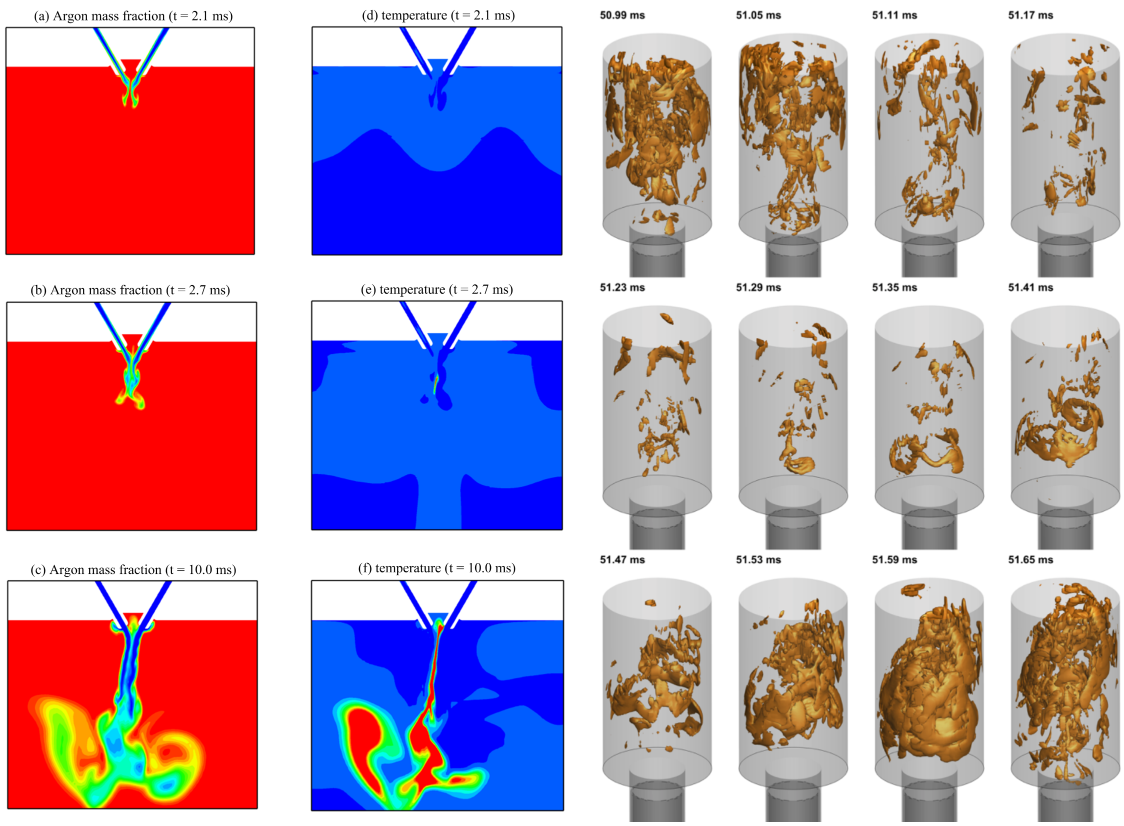

Figure 1. (a) Left: Argon mass fraction and temperature contours for gas-phase ignition transients if mono-methyl hydrazine and red fuming nitric acid propellants. From Sardeshmukh *et al.*[7] (b) Right: Heat release iso-surfaces for one acoustic cycle of an unstable methane-hydrogen-peroxide rocket combustor. From Harvazinski *et al.*[8]

Our interest in unsteady dynamics naturally requires the use of turbulence models that are capable of representing fine-scale time-dependent phenomena. Direct numerical simulations are, of course, well beyond reach for the high Reynolds number conditions that are encountered in aerospace propulsion problems. We therefore focus on large eddy simulations (LES)[1] and detached eddy simulations (DES)[2] models in this paper. DES models are a member of the larger class of hybrid RANS/LES models, where RANS (or Reynolds-averaged Navier-Stokes) equations are solved in the near-wall boundary layer region, while LES equations are solved in the off-body region. Such hybrid models are popular in engineering codes mainly because of the computational savings enabled by the near-wall RANS model, while full LES models are more commonly utilized in academic codes and applied to canonical problems. We further note that unsteady RANS (URANS) models are sometimes utilized for time-dependent problems. However, such an approach is valid only if the unsteady time-scales are well removed from the turbulent time-scales, which is generally not true for the applications of interest here. We therefore do not consider traditional RANS or URANS models. In our study, we start with the filtered conservation laws in compressible form as the basic set of equations to be solved. These equations contain unclosed terms such as the turbulent stress and scalar-velocity covariance terms that are defined by the LES turbulence models, traditionally, by using an eddy viscosity/gradient diffusion hypothesis. These closures are also referred to as sub-grid models in the sense that they represent the net effect of the unresolved flowfield fluctuations.

Turbulent combustion models are used to close the filtered combustion source terms that appear in the species transport equations. Three classes of models are considered here: the steady laminar flamelet model,[3] the linear eddy model (LEM)[4,5] and the transported-probability distribution function (PDF) method.[6] We note that many of these models also provide a means for replacing the direct solution of the species transport equations, which allows for significant simplifications of the combustion model itself. A prominent example is the steady laminar flamelet model wherein the chemistry is tabulated in terms of a small number of transported variables such as the mixture fraction and/or one or more reaction progress variables. In the case of the transported-PDF model, the solution of the joint-PDF of the chemical composition of the propellant mixture also eliminates the need for a separate solution of the species transport equations in the Eulerian framework. Likewise, the LEM approach treats the species transport equation in a Lagrangian manner. Such model attributes make it difficult to compare the different models fairly since each model is essentially designed to accomplish different aspects of the overall turbulent combustion problem. As discussed earlier, our approach in the current evaluation is to use the filtered conservation laws as the basic set of equations to be solved and the turbulent combustion models then provide the basis for modeling the unclosed terms, i.e., the filtered combustion source terms. In other woods, the role of the turbulent combustion closure is strictly to provide sub-grid models to capture the effects of the unresolved fluctuating flowfield on the combustion.

The key aspect of this study is the evaluation of the fundamental model assumptions underlying the turbulence and turbulent combustion models. The traditional LES and DES turbulence models are gradient-diffusion models which have inherent difficulties representing physical phenomena such as back-scatter. We note that back-scatter is recognized as being significant even in non-reacting flows[9,10] and it is likely that these effects are more significant in turbulent combustion because the combustion heat release can occur in scales that are smaller than the smallest turbulent scales. Further, we attempt to shed some light on the issue of the grid resolution required for LES and also examine the inter-relationship of numerical errors with sub-grid modeling errors. A major limitation of turbulent combustion models as pertains to aerospace propulsion applications is that they are typically derived for low-Mach combustion. This calls into question their validity for representing fundamentally compressible phenomena such as shocks and/or acoustics. Moreover, many turbulent combustion models are selectively formulated for certain regimes such as the flamelet regime or for certain types of combustion such as premixed or non-premixed. Aeropropulsion problems often involve multiple turbulent combustion regimes ranging from non-premixed through partially premixed and all the way to fully premixed in a single flowfield. This again challenges the basic assumptions of the models. Thus, in each of the model description sections, we also carefully evaluate the basic model assumptions and document the applicability of the models. Furthermore, as noted earlier, we view the different sub-grid models as closures of the full set of conservation laws, thereby enabling these models to be compared on a more equal footing.

The outline of the paper is as follows. We begin by presenting the filtered LES transport equations for mass, momentum, energy and species. We then present the basic formulation of the constant and dynamic Smagorinsky models and discuss their fundamental assumptions and limitations. This is followed by the formulation of the steady flamelets, linear eddy model and the transported-PDF model. In each case, we again provide a detailed evaluation of the model assumptions and how they might impact our ability to address some of the unique aspects of aerospace propulsion flowfields. Finally, we provide some conclusions and suggest directions for future work.

II. Equations of Motion

The conservation laws for mass, momentum, energy and species transport expressed in Favre-filtered form for LES computations are:[11]

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{u}_i) + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{u}_j\widetilde{u}_i) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\overline{\tau}_{ji} - \overline{\rho}\left(\widetilde{u_j u_i} - \widetilde{u}_j\widetilde{u}_i\right)\right] \tag{2}$$

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{h}_0\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{h}_0\right) = \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_j}\left(\widetilde{u}_i\overline{\tau_{ij}} - \overline{q}_i + \left(\widetilde{u_i\tau_{ij}} - \widetilde{u}_i\overline{\tau_{ij}}\right) - \overline{\rho}\left(\widetilde{u_j h_0} - \widetilde{u}_j\widetilde{h}_0\right)\right) \tag{3}$$

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{Y}_l) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{Y}_l\right) = \overline{\dot{\omega}}_l + \frac{\partial}{\partial x_j}\left[-\overline{\rho}\widetilde{V}_{l,j}\widetilde{Y}_l + \overline{\rho}\left(\widetilde{u_j Y_l} - \widetilde{u}_j\widetilde{Y}_l\right)\right] \tag{4}$$

Favre-filtering is defined as $\tilde{u} = \overline{\rho u}/\overline{\rho}$, where the over-bars refer to conventional filtering of the density and density-velocity product. A detailed derivation of the filtering process including a discussion of the role of commuting filters is given by Oefelein.[12]

Two sets of terms in the above equations require closure. The first are the velocity-velocity (turbulent stresses) and scalar-velocity covariance terms of the form, $\overline{\rho}\left(\widetilde{u_j\phi} - \widetilde{u}_j\widetilde{\phi}\right)$, which appear as the last two terms in the momentum, energy and species transport equations respectively. The second set of terms requiring modeling is the combustion source terms which typically take the highly non-linear form of Arrhenius expressions. For LES, the covariance terms may be expanded as:[13]

$$\overline{\rho}\left(\widetilde{u_j\phi} - \widetilde{u}_j\widetilde{\phi}\right) = \underbrace{\overline{\rho}\left(\widetilde{\widetilde{u}_j\widetilde{\phi}} - \widetilde{u}_j\widetilde{\phi}\right)}_{\text{Leonard stress}} + \underbrace{\overline{\rho}\left(\widetilde{\widetilde{u}_j\phi''} + \widetilde{u''_j\widetilde{\phi}}\right)}_{\text{Cross-term stress}} + \underbrace{\overline{\rho}\widetilde{u''_j\phi''}}_{\text{Reynolds stress}} \tag{5}$$

The specific covariance term with $\phi = u_i$ is typically denoted as the sub-grid scale stress, τ_{ij}^{sgs}. Leonard stresses appear in closed form and do not need to be modeled. It is worth noting that these terms account for interactions between resolved scales, while the cross terms involve interactions between resolved and unresolved scales.[12] One may then speculate that the cross-stress terms would account for the bulk of the inter-scale energy transfer including the back-scatter phenomenon. On the other hand, the Reynolds stresses account for interactions only between the unresolved scales. Finally, we note that both the cross-stress terms and the Reynolds stress terms are not closed and require modeling as do the combustion source terms. These models are discussed in the following sections.

III. Turbulence Models

The most popular LES closure is the Smagorinsky model and is considered here both in its original constant form[14] and in the later dynamic version.[15,16] We note that fundamental to LES is the idea of scale-similarity in the inertial sub-range, a fact that is utilized in the formulation of the dynamic procedure as discussed later. Two classes of LES filter models can be categorized: implicit filtering, in which the grid size and filter width are the same and no actual filtering of the solution is performed, and explicit filtering, wherein the grid size is smaller than the filter-width and the solution is filtered at each time-step using the filter size. It should be observed that this means that explicit filtering typically requires the use of finer grids, which would naturally lead to better solutions, but not necessarily due to the explicit filtering operation. Most of the following discussion is common to both classes of models although implicit filtering is assumed unless otherwise specified.

In both sets of models, the Reynolds stress term is first expressed as the sum of the deviatoric and isotropic stress parts. The deviatoric part is given by:

$$\tau_{ij}^{D,sgs} \equiv \tau_{ij}^{sgs} - \frac{1}{3}\tau_{ii}^{sgs}\delta_{ij} \tag{6}$$

where τ_{ij}^{sgs} is the Reynolds stress defined above. The isotropic part of the stress is:

$$\tau_{ij}^{I,sgs} \equiv \frac{1}{3}\tau_{ii}^{sgs}\delta_{ij} \tag{7}$$

The deviatoric part is modeled as

$$\tau_{ij}^{D,sgs} = -2\nu_t \overline{S}_{ij} \tag{8}$$

where $^-$ signifies application of a filter.

In the constant Smagorinsky model, the turbulent eddy viscosity, ν_t, is modeled as

$$\nu_t = C_s \Delta_g^2 \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2} \tag{9}$$

where length scale, is taken to be proportional to the filter or grid width Δ_g with a proportionality constant C_s, the Smagorinsky coefficient.

In the dynamic Smagorinsky model, Germano *et al.*[15] proposed a method whereby C_s is determined as the calculation progresses instead of specifying it *a priori.* The associated eddy viscosity is given by:

$$\nu_t = C(x,t)\Delta_g^2 \left|\overline{S}\right| \tag{10}$$

where $C(x,t)$ is the dynamic Smagorinsky coefficient and $\overline{S} = \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2}$. A procedure for solving for C proposed by Lilly[16] involves the application of a test filter of width Δ_t with a scale larger than the grid filter width, Δ_g, i.e., $\Delta_t = a\Delta_g$ and $a > 1$. The dynamic model thus incorporates local instantaneous information about the strain-rate field at the smallest resolved scales to determine a value of C that varies continuously in space and time throughout the simulation.

The isotropic part of the stress tensor is modeled as:

$$\tau_{ij}^{I,sgs} = 2C_I \Delta_g^2 |\overline{S}|^2 \tag{11}$$

where C_I is a dimensionless coefficient.[12] Similar expressions may be written for the sub-grid-scale energy and species fluxes using the standard gradient diffusion hypothesis.

The idea of scale similarity is key to LES models. This means that it is important to ensure that the grid size is adequate for the resolved turbulence field to be within the inertial sub-range. An often-used condition is the so-called Pope's criterion that stipulates that the grid must be able to resolve at least 80% of the total energy.[17] This is, however, not a rigorously derived criterion and is one that is difficult to check precisely since the total energy content for a given problem is typically not known. An easier check would be to verify the degree of isotropy in the velocity field. A related issue has to do with the grid size required to resolve a certain cut-off wavenumber in the inertial sub-range. It is common practice to select the grid size to be equal to the reciprocal of the cut-off wavenumber, which means that the smallest resolved scale is being captured with only one or two grid points. Clearly, this is insufficient resolution. In fact, the number of grid points required to capture a certain turbulent scale is highly scheme-dependent since it is dependent on the damping and dispersion characteristics of the scheme. In general, second-order accurate schemes would require of the order of 10-20 points across the smallest resolved scale to properly capture the energy contained in that scale. Higher-order schemes require substantially fewer grid points, but conventional finite-difference and finite-volume schemes still need some seven or eight grid points at the minimum.

From the above discussions, it is clear that if adequate grid resolution is not provided and the same grid is used by different codes, the resulting solutions would be code- (or scheme-) dependent. In fact, this has been observed by many researchers (see Cocks *et al.*[18] for a recent example) and has been attributed to the impact of numerical errors on the physical accuracy of LES schemes. While the latter observation is certainly true, we note that it is based on the assumption that the same grid would work equivalently for different schemes or different code implementations. The important (and obvious) conclusion that should be drawn is that the necessary grid size for adequate LES resolution is dependent on the order of accuracy of the scheme and even on the particular implementation details. In fact, with adequate grid resolution we expect that grid-convergence of the main statistical quantities would be attained. We also note that these observations are true for both implicit-filtering and explicit-filtering, although in the latter case, the use of finer grids would likely move the solutions into the acceptable realm.

It is well established that back-scatter is a common phenomenon even in non-reacting turbulent flows. Back-scatter refers to the effect of locally transferring energy from the small to large scales. For instance, Piomelli *et al.*[9] have found that backscatter occurs at nearly half the points at any given time instant in a flow and that the net energy transfer (which is equal to the sub-grid scale dissipation) is the difference between two large quantities: i.e., the energy transfer from large to small scales and the backscatter. The authors

also speculate that, for non-equilibrium flows, this effect could be even stronger. Combustion problems wherein the energy deposition often occurs in the smallest scales (even smaller than the Kolmogorov scale) may well represent such a case. It is therefore critical that the LES sub-grid models are capable of properly representing back-scatter phenomena. It has been pointed out that the dynamic Smagorinsky model can predict back-scatter since the eddy viscosity can be negative during certain instances in time.[15] However, since the Smagorinsky model is essentially based on Prandtl's mixing length model, its natural ability to represent inter-scale energy transfers is questionable. It would seem likely that more sophisticated sub-grid models employing the transport of the sub-grid turbulent kinetic energy and/or the length scale would be a better approach towards improved LES predictive capability. Such approaches have been proposed in the literature by Schumann[19] and have been extended to use dynamic coefficients by Menon and his co-workers.[20] As a further comment, we point out that the use of negative eddy viscosity to represent back-scatter may well be physically incorrect because of the fundamental stability implications of such a formulation. Besides, a negative eddy viscosity coefficient does not have a clear physical interpretation with regard to turbulent flow. It may be more appropriate to look at the modeling of the cross-stress terms in the LES equations to provide the correct unresolved-to-resolved scale interactions.

An alternate approach to the closure problem is the detached eddy simulation or DES model pioneered by Spalart and his colleagues.[2,21] As noted earlier, the DES is a hybrid RANS/LES model, wherein the RANS equations are solved in the near-wall region and the LES model is applied to only the off-body regions. Such hybrid models operate more efficiently because of the reduced grid count and are popular in engineering CFD codes. A major issue that arises with these methods, however, is the fundamental inconsistency in the definition of the sub-grid quantities in the two models. For instance, the turbulent kinetic energy represents the energy in the entire fluctuating field in the RANS regions, while it represents only the sub-grid contributions in the LES regions. Appropriate matching procedures must be specified in the overlap region between the RANS and LES models, but this aspect is usually ignored in most implementations (see Xiao *et al.*[22] for an interesting exception).

A final comment that we make with regard to LES models relates to the use of the gradient diffusion hypothesis, which is at the core of most standard LES closures. In addition to possible ambiguities that arise with respect to representing the back-scatter phenomena correctly, it has been suggested that the use of the gradient diffusion model in the species transport equation when sources are present leads to fundamental contradictions (e.g., see Peters[3]). It is sometimes argued that the determination of variable turbulent Schmidt numbers using the Germano scale similarity ideas would introduce such effects correctly, but such observations have not been rigorously substantiated in the literature. Another interesting observation is that velocity-composition PDF methods provide a non-gradient-diffusion-based closure to the covariance terms in the momentum, energy and species equations.[6] An interesting speculation is whether or not PDF methods could shed some light on the importance and sensitivity of some of these effects.

IV. Turbulent Combustion Closure Models

Numerous approaches have been proposed for the closure of the turbulent combustion source terms in the filtered conservation equations.[3–6,11,23] Table 1 lists the main classes of models, along with the key assumptions and the solution process in each case. Some models such as the linear eddy model (LEM) solve the full set of transport equations—continuity, momentum, energy and species—and attempt to model only the sub-grid terms. On the other hand, models such as flamelets and transported probability density function (PDF) or the related filtered mass density function (FMDF) models involve additional assumptions such as the modeling of the combustion kinetics (in flamelets) or scalar mixing (in PDF or FMDF methods).

A recurring approximation that appears in some form in nearly all the turbulent combustion models is the limitation to low Mach numbers. This approximation uncouples the hydrodynamic equations (continuity and momentum) from the composition equations (energy and species) so that each can be solved as a separate set. In the low Mach number approximation, the hydrodynamic equations impose a constant mean pressure upon the composition equations enabling the density to be obtained from the enthalpy and species mass fractions without involving the velocity. Transmitting this density to the hydrodynamic equations enables the latter system to be closed as well. The low Mach number assumption has its roots in steady RANS modeling where pressure variations scale with the square of the Mach number. The approximation becomes somewhat more restrictive in unsteady problems where pressure variations scale with the first power of Mach number, but is likely unacceptable in fully compressible applications. In keeping with the philosophy of this

Table 1. Turbulent Combustion Models

Model	Key Assumptions	Procedure	Validity
Flamelets (Non-premixed) G-Equation (Premixed)	1D, steady laminar velocity field Equal diffusion coefficents Presumed PDF Low Mach	Solves for Z, Z" Reaction progress variable Tabulated reactive scalar solutions Derive filtered quantities	Low Mach High Da Low Re
LEM Premixed/ Non-premixed	Sub-grid transport model 1D, constant pressure in sub-grid Exact combustion closure	Species convection in LES grid 1D reaction-diffusion in LEM grid Explicit LEM solution	All regimes
PDF-Transport Premixed/ Non-premixed	Exact combustion closure Exact covariances Scalar mixing model Low Mach assumption	Hybrid Lagrangian/Monte Carlo/ Deterministic solution Reactions coupled with subgrid (or ISAT)	Low Mach All Da All Re

paper, however, we note that it is possible to solve the full set of equations and model only the sub-grid terms with nearly any turbulent combustion model although, again, it may not be possible to use the low Mach number approximation in any fashion for the applications at hand.

IV.A. Steady Flamelet Models

The so-called flamelet approximation involves the assumption that non-equilibrium effects are restricted to the immediate vicinity of the flamefront, which is justifiable when the time-scales of the chemistry mechanisms are smaller than the smallest turbulent scales.[3] Flamelet models replace the large number of reactive scalar equations by a single (or a few) conserved scalar equation(s). For example, a mixture-fraction equation representing the mixing between fuel and oxidizer streams can be written in Favre-filtered form as:

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{Z}) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{Z}\right) = \frac{\partial}{\partial x_j}\left[\overline{\rho D}\frac{\partial}{\partial x_i}\widetilde{Z} + \overline{\rho}\left(\widetilde{u_j Z} - \widetilde{u}_j\widetilde{Z}\right)\right] \tag{12}$$

The conserved scalar equation has the attractive advantage that it contains no source terms although its derivation involves a number of approximations. Key among these are an assumption of equal mass diffusivities in the species equations and a unity Lewis number in the energy equation along with the low Mach number assumptions of constant pressure and the neglect of viscous dissipation. Clearly, many of the latter assumptions are invalid for compressible flows and, in particular, solving the conserved scalar equation in lieu of the full energy equation will result in the wrong sound speed. Thus, unsteady shock phenomena and acoustics propagation will be incorrectly captured. For this reason, it is necessary to retain the full form of the energy equation for the compressible problems of relevance here.

The key feature of the flamelet approach lies in the tabulation of the chemistry such that the solution of the above conserved scalar equation allows the determination of the individual species mass fractions. In the basic steady flamelet model, the reactive scalar compositions are parametrized in terms of the conserved scalar function and the scalar dissipation rate, χ, and the associated flamelet equations are written in one-dimensional form as:

$$\frac{\rho}{2}\chi\frac{\partial^2\psi_i}{\partial Z^2} + w_i = 0 \tag{13}$$

where Z is the conserved scalar variable and ψ_i is the reactive scalar variable, which represents the vector $(Y_i, T)^T$. Also, χ is the scalar dissipation rate which typically reflects the role of varying the strain rate on the flame. The key approximations in the derivation and solution of the flamelet equations are: (1) the pressure in the reactive scalar system is approximated as a constant (low Mach number assumption), (2) the velocity field is specified from a simplified problem (such as counter-flow diffusion flames) rather than from the actual flow-field solution, and (3) the entire set of species equations is solved in conjunction with an approximate form of the energy equation.

The representative solution is obtained analytically or numerically for a model problem, parameterized by the mixture fraction and the scalar dissipation rate and then tabulated for efficient look-up:

$$\psi_i = \psi_i(Z, \chi_{st}) \tag{14}$$

Typical model problems usually take the form of a simple canonical configuration such as a premixed flame or a counterflow diffusion flame.[3] In neither case is the underlying velocity field in any way related to the actual velocity field in the real problem. Naturally, this assumption eliminates the influence of non-equilibrium phenomena such as turbulence, acoustic waves and shock or vortex interactions. Further, the canonical problem is typically expressed in terms of adiabatic reactions between fuel and oxidizer at the inlet temperature, as opposed to mid-flame reactions where the reactants may be preheated or partially reacted/decomposed. Similarly near wall regions may experience significant heat loss. Some of these effects can be incorporated by expanding the model problem tabulations to include multiple inlet temperatures, species radicals and heat losses although the complexity increases rapidly. Limited attempts at such approaches have been made, but it is hard to capture all the effects that define unsteady flowfields such as those illustrated in Figs. 1 (a) and (b). Further, the simultaneous presence of premixed, non-premixed and partially premixed combustion within the same physical problem also complicates the application of flamelet tables since decisions need to be made regarding which table is relevant in each region. Efforts to extend the validity of the model to represent dynamic phenomena such as ignition and extinction include Moin and Pierce[24] who originally introduced a reaction progress variable in combination with the steady flamelet equation. Recent progress using the unsteady flamelet equations is due to Pitsch, Ihme and their colleagues.[25,26]

The assumption of laminar flamelets is strictly justified only in the small Karlovitz (Ka) number limit, i.e., when the chemistry scales are much smaller than the Kolmogorov scales. Alternately, this limit may be expressed in terms of the Damkohler (Da) number, which is the ratio of the turbulent time scale to the chemical time scale, as shown in Table 1. In the high-Da limit lies the traditional thin flamelet regime. However, in the presence of slow reactions such as pyrolysis and/or at high Reynolds numbers that lead to smaller turbulent scales, we enter the distributed or broken reaction zone which is not well captured by the flamelet assumption. In fact, under such low-Da conditions, the importance of turbulence interactions dominating the laminar flamelet solution should not be ignored. A possible approach is to define an appropriate number of additional reaction progress variables to further enrich the tabulated chemistry, but to our knowledge, a systematic study of such ideas in the context of distributed combustion zones has not been performed.

Perhaps a more fundamental assumption of such a generalized tabulated chemistry approach is that a reduced representation of a large-dimensional manifold by a lower-dimensional manifold (say with two dimensions, namely the conserved scalar and a reaction progress variable) is always possible, unique and accurate. Pope has argued that accuracy of the low-dimensional manifold representation is only modestly improved by small increases in the number of dimensions, say from two to three, and that as many as 6-8 dimensions (or reaction progress variables) may be required to accurately capture the full manifold space.[27] Naturally, this introduces fundamental challenges to the generality of the tabulated chemistry approach and would necessitate the use of in-situ adaptive procedures for such a large-dimensional table generation and storage.

The discussion so far has been limited to the representation of the chemistry by the flamelet or tabulated approach. Once the reactive scalars are obtained, they need to be appropriately filtered (or averaged) to calculated the mixture density. This can be expressed using a joint-presumed probability density function (PDF) for Z and χ_{st}:

$$\tilde{\psi}_i(x,t) = \int_0^1 \int_0^\infty \psi_i(Z,t,\chi_{st}) \tilde{P}(Z,\chi_{st};x,t) d\chi_{st} dZ \tag{15}$$

The presumed PDF is usually expressed by assuming statistical independence of Z and χ_{st} with the PDF of Z being taken as a beta function[3] parameterized by the variance of the conserved scalar function, Z''. The mixture fraction variance is then obtained by solving an appropriate transport equation. This assumed PDF shape contrasts with the more rigorous computed distribution functions used in LEM and transported-PDF methods that are founded upon more physics-based approaches. While the flamelet model constitutes an efficient combustion solution method its application to turbulent combustion relies solely upon the presumed PDF. In looking toward applications in which turbulent combustion closures are incorporated into the filtered conservation equations presented in Section II, the presumed PDF would appear to be a significant handicap to accurate predictions. Moreover, it is clearly possible to compute the PDF with either LEM or PDF and use a flamelet model for the combustion, thereby bypassing the assumed PDF.

IV.B. Linear Eddy Model

In contrast to flamelets, the LEM approach solves the complete set of conservation equations.[4,5,20] However, only the continuity, momentum and energy equations are solved in filtered form on the global (LES) scale, while the species transport equations are solved in unfiltered form using a multi-scale approach. The overall solution procedure is as follows. First, the LES equations are solved for the velocity, density and energy components of the flow. The unfiltered form of the specifies equation is written as:

$$\rho \frac{\partial Y_k}{\partial t} + \rho u_j \frac{\partial Y_k}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho V_{j,k} Y_k\right) + \dot{w}_k \tag{16}$$

where V_{jk} is the diffusion velocity and $\dot{w}_k$ is the species production and destruction term. We write the convective term of the above equation in a slightly different form:

$$\rho \frac{\partial Y_k}{\partial t} + \rho\left(\tilde{u}_j + (u_j')^R + (u_j')^S\right) \frac{\partial Y_k}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho V_{j,k} Y_k\right) + \dot{w}_k \tag{17}$$

where we have substituted for the unfiltered velocity in terms of the filtered velocity field ($\tilde{u}_j$), the LES-resolved sub-grid fluctuation ($u_j^{'R}$) and the unresolved sub-grid fluctuation ($u_j^{'S}$).

In the so-called LES-LEM model, this equation is further split into two parts. The first part is a sub-grid part, comprised of the sub-grid mixing, diffusion and chemical source term, while the second is a large-scale advective part. Thus:

$$Y_k^* - Y_k^n = \int_t^{t+\Delta t_{LES}} -\frac{1}{\rho}\left(\rho (u_j')^S \frac{\partial Y_k^n}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\rho V_{j,k} Y_k\right)^n - \dot{w}_k\right) dt \tag{18}$$

$$Y_k^{n+1} - Y_k^* = -\Delta t_{LES}\left(\tilde{u}_j + (u_j')^R\right) \frac{\partial Y_k^n}{\partial x_j} \tag{19}$$

The sub-grid species solution is accompanied by the low Mach number form of the thermal energy equation in order to capture the sub-grid heat release and the composition field. (Note that LEM uses the full energy equation on the LES grid so that the low Mach number approximations appear only on the sub-grid. As a consequence, LEM has two temperature fields; an approximate one that is used on the subgrid, and a complete one that is on the LES grid. A similar situation arises with flamelets and transported-PDF methods when the full form of the energy equation is solved in the resolved scale.) The sub-grid solution is obtained from a set of one-dimensional equations aligned in a direction normal to the maximum gradient of the species mass fraction. It is comprised of three terms. The first term is the advective mixing term that is modeled using stochastic rearrangement events called triplet maps, which model the effects of sub-grid eddies of specified size, location and frequency.[4] The second term represents molecular diffusion and is solved using explicit time-stepping in the 1D LEM grid. The third term is the combustion source term, which is typically integrated using an ODE solver. Finally, the large-scale advective solution is carried out using a Lagrangian approach and involves splicing and regridding (of the 1D LEM grid) operations to account for mass transfers between LES cells and volumetric expansion due to combustion. In principle, the LEM model is applicable for all flow and combustion regimes because it makes no assumptions of scale separation between combustion and turbulence.

There are some issues with the LEM approach. The first has to do with the fact that the large scale advection equation contains no diffusion. Therefore, while diffusion is properly represented in the LEM grid, there is no species diffusion in the LES grid. This is an important issue for a number of reasons. For one, the dissipation range is usually not restricted just to the Kolmogorov scales and can extend well into the inertial range as well. Secondly, in the limit of fine-grid resolution (say in the vicinity of walls), the LES grid itself may approach the Kolmogorov length scale. In that limit, the LEM grid may be reduced to a single node or just a few nodes and the lack of diffusion in the LES grid would render the solution incorrect. Proposals have been made to include a diffusion term in large-scale advective solution or, alternately, to use a hybrid approach wherein the LEM is only active for those regions that are away from the diffusion range. However, to our knowledge, these methods are yet to be rigorously assessed.

The large-scale advective solution also introduces a second difficulty into the LEM method. As discussed above, a Lagrangian method is used to transport the species between the LES grid cells. This is done by looking at the sign of the wall normal velocity at the cell-face in order to determine if the species transport

is occurring to the cell or away from the cell. This 'splicing' procedure involves cutting off pieces of the 1D LEM strand and transferring them to the neighboring cells. The main difficulty with this approach is that the order of species transport between cells is arbitrary. As a result, there is a certain randomness to how this redistribution is carried out and, moreover, the resulting LEM strands may have very noisy solutions. It is unclear how this discrepancy can be resolved within a Lagrangian method, although a simple correction would be to use the Eulerian form of the species transport equation for the large-scale transport. Again, this would mean using the full set of filtered conservation laws given in Section II and the LEM solution would then become simply a means to close the turbulent combustion source term in these equations.

A final issue has to do with the assumption of constant pressure in performing the LEM sub-grid solution. Obviously, this has limitations for capturing compressible phenomena within the sub-grid. There is a need to devise a more rigorous method to formulate the sub-grid problem so that the compressible fluid-dynamics equations can be correctly represented in the sub-grid solution. A potentially interesting complement/upgrade to LEM methods is the one-dimensional turbulence (ODT) approach.[28,29] ODT can be viewed as an extension of LEM to includes analogous sub-grid modeling for the velocity components as well as the composition variables. It offers the possibility of incorporating more fundamental turbulence modeling in the LEM format, but further development is needed to apply ODT in practical propulsion applications.

IV.C. Transported-PDF Models

Transported PDF methods use a one-point, one-time joint PDF of a set of flow variables to model the dominant non-linear effects in turbulent combustion.[6,30–32] Although simpler formulations have been implemented, the joint PDF in current state-of-the-art applications incorporates velocity, turbulence frequency and composition variables. The present discussion will focus on this set. The most compelling feature of PDF methods is that they can exactly represent the thermochemical source terms in the species equations. These source terms are independent of adjacent locations in both space and time and so are ideally represented by a one-point, one-time PDF approach. Further, radiation emission can similarly be represented exactly[30] thereby offering a path toward modeling additional physics in practical combustion problems.

The velocity-frequency-composition joint PDF also enables convection and the resulting Reynolds stress and velocity-scalar co-variance terms to be represented exactly. To accomplish this, the equations are expressed in substantial derivative form and evaluated in a Lagrangian sense. PDF methods therefore provide an interesting contrast to gradient diffusion models used in traditional approaches. It has been argued that gradient diffusion is appropriate only for equations without source terms.[3,33] Flamelet remove the sources in the scalar equations by the mixture fraction approximation thereby making the gradient diffusion approximation valid. PDF methods solve scalar equations with source terms but avoid gradient diffusion by representing the co-variance terms exactly. An advantage of the co-variance representation in PDF methods is that it should allow back-scatter whereas it is unclear that gradient diffusion models can correctly represent it.

Although these crucial turbulence-combustion interaction terms can be represented exactly, PDF models require modeling for the remaining quantities. The dominant process that must be modeled in the classical low Mach combustion regime is molecular diffusion. Mixing models have received considerable attention,[33–36] with emphasis on non-premixed and partially premixed applications. The PDF equations, however, are equally applicable to premixed and partially premixed problems in all Damkohler regimes and extensions to mixing models for these regimes are on-going. The transported PDF equation is written as:

$$\begin{aligned}
<\rho> \frac{\partial \tilde{f}}{\partial t} + <\rho> V_j \frac{\partial \tilde{f}}{\partial x_j} - \frac{\partial <p>}{\partial x_j} \frac{\partial \tilde{f}}{\partial V_j} + \frac{\partial}{\partial \psi_k}\left(<\rho> S_k \tilde{f}\right) \\
= \frac{\partial}{\partial V_j}\left(\left\langle -\frac{\partial \tau_{ij}}{\partial x_i} + \frac{\partial p'}{\partial x_j}(V,\psi)\right\rangle\right)\tilde{f} + \frac{\partial}{\partial \psi_k}\left(\left\langle \frac{\partial J_i^\alpha}{\partial x_i}(V,\psi)\right\rangle\right) \qquad (20)
\end{aligned}$$

The terms on the left include acceleration in physical, velocity and composition space and are represented exactly assuming that the volume-averaged pressure gradient is known. The terms on the right include viscous effects, fluctuating pressure gradients and molecular diffusion, all of which involve conditional probabilities and must be modeled.

From a practical viewpoint, the most significant disadvantage of the PDF approach is the dimensionality of the transport equation which involves a total of NS + 8 independent variables for the velocity-frequency-

composition PDF. With this large number of independent variables, finite element/volume methods are impractical and particle-based, Monte Carlo methods become imperative. Typically, the flow is represented by a Lagrangian set of particles that evolve on the basis of stochastic differential equations in which the properties of each particle depend on its mass, physical coordinates, velocity, composition and turbulence frequency.[6]

An additional issue with Eqn. 21 is that the velocity-frequency-composition PDF constitutes an unclosed system. The solution of the PDF equation requires the instantaneous pressure while the mean pressure appears as a coefficient in the exact terms on the left side. This difficulty is traditionally bypassed by invoking the low Mach number assumption to split the hydrodynamics from the composition variables as is done in the flamelet (and to a lesser extent in LEM) approaches. The low Mach number approximation relegates the instantaneous pressure to a constant impressed upon the fluctuating fields by an external mean while the mean pressure is obtained from a hydrodynamic code. The low Mach number form of the equation of state is enabling to this variables split since a constant pressure implies that density can be obtained directly from species mass fractions and temperature. PDF methods therefore invariably involve hybrid methods containing both stochastic (transport equation) and deterministic (hydrodynamic conservation equation selected from Eqns. 1-4).

The simplest procedure for obtaining the mean pressure is to use a Poisson equation for the pressure obtained by taking the divergence of the momentum equations. The mean pressure is then obtained from an external field solver while the fluctuating (and mean) velocity, composition, enthalpy and turbulence frequency are obtained from the PDF. The implementation of this so-called stand-alone method is problematic due to scatter from stochastic fluctuations in the PDF solver.[6,37] A more practical approach is to use a hybrid method that solves the filtered continuity, momentum and enthalpy equations (Eqn. 1 and 2 and a low Mach number version of Eqn. 3) by field methods while using a velocity-composition-frequency joint PDF to obtain the density and turbulence quantities. The two portions of the calculation are then coupled by sending mean pressure, velocity and enthalpy fields to the PDF solution while the PDF solution transmits the mean density and turbulence quantities to the field solver. The low Mach number form of the equation of state is again necessary for accomplishing this variables split. In addition to using deterministic mean quantities to suppress difficulties in the field solution, their use as coefficients in the SDEs of the PDF solution also improves their behavior. Although such hybrid methods introduce multiple duplicate fields whose consistency has to be assured,[38] they are an order of magnitude faster than the stand-alone method that uses only the pressure Poisson equation for the mean pressure, and which is fraught with instabilities and errors arising from statistical variations.[37]

In the present paper where we are interested in extending turbulent combustion models (and, in this section, PDF models) to compressible flows with ensuing high Mach number effects and acoustic fluctuations, it is pertinent to speculate on the research that must be addressed to model these new regimes. As with the flamelet-like models, the first issue is a procedure for bypassing the common separation of the hydrodynamic equations (continuity and momentum) from the composition variables (species and enthalpy) by means of a spatially constant mean pressure. Similarly, the exact equation of state must be invoked as opposed to its constant pressure approximation. Dropping these low Mach number approximations implies that the complete system (hydrodynamic and composition variables) is fully and intimately coupled. Initial efforts in this direction have extended the joint PDF to include pressure in addition to velocity, enthalpy, species mass fractions and frequency. With pressure (or, more generally, two thermodynamic variables) included, the joint PDF can, in principle, be solved independently without a companion field equation code.[39,40] The pressure evolution equation in this approach is entirely modeled with the pressure strain rate correlation taken from second order turbulence models.[41–43] In addition, a compressible approach for isentropic flows (pressure and density algebraically related by an isentropic relation) has also been outlined.[44]

While it is possible to obtain the entire flowfield solution from a PDF equation without the use of field equations, experience with the PDF/Poisson solver suggests that it is likely that a better implementation would couple the pressure-velocity-frequency-composition PDF with the deterministic mean equations (i.e., Eqs. 1-4). Such a procedure will require that the intimate coupling between composition and hydrodynamic variables that occurs in compressible flows be realized in both the stochastic and the deterministic portions of the model. One such result has been reported[45] in which a conventional finite volume code was coupled with a composition PDF formulation. Apart from this, there appears to be no examples of using hybrid finite volume/PDF methods for compressible flows. It would appear that incorporation of deterministic models for the mean quantities should, at least, be evaluated. Applying the philosophy stated at the outset

of the paper, a possible approach would include using a pressure-enthalpy-velocity-species-frequency joint PDF to compute the co-variance terms in the momentum, energy and species equations and the source term in the species equations. These turbulence quantities could then be supplied to a finite volume solver as a representation of non-linear effects thereby enabling the filtered LES equations to be solved in fully coupled form. The large-scale properties could then be transferred to the PDF solver to provide smooth coefficients for improved stochastic characteristics. Ensuring consistency between the two solvers would be an important issue, but much of the current advances could be adapted.

A final comment concerning a completely different approach to turbulent combustion modeling is in order. The thickened flame approximation,[11] originally applied to premixed combustion has been used for non-premixed combustion problems involving combustion-acoustic interactions.[46,47] The thickened flame approximation allows the fully coupled nature of the equations that is characteristic of flows with compressibility effects and acoustic-turbulence coupling to be immediately resolved by classical compressible flow algorithms. Thus while the thickened flame approximation may be somewhat lacking in rigor, it enables acoustic/compressibility effects to be treated directly. To the authors' knowledge, this is the only turbulent combustion model that has been applied to compressible combustion problems with acoustic interactions.

V. Conclusions and Future Study

A fundamental evaluation study of state-of-the-art turbulence and turbulent combustion models of relevance to aerospace propulsion applications is undertaken. Our interest is in evaluating the ability of the models to capture physical phenomena related to high-speed flows, high pressures, ignition behavior, shocks and acoustics interactions. Such problems occur frequently during off-design operation of propulsion systems and are responsible for test failures and expensive re-designs in any development program. In addition to shedding light on the strengths and limitations of the methods, we hope to identify paths for future study in these challenging areas.

The framework that we use to undertake this study consists of the full conservation laws for mass, momentum, energy and species transport. In filtered form, these equations contain a number of unclosed terms, namely the Reynolds stresses, and associated co-variances of the velocity, enthalpy and species. In addition, the combustion source term appears unclosed in this version of the equations. For the sake of consistency in the evaluation, we regard the different models as specific attempts to close one or more of these terms. In other words, the turbulence models close the turbulent stress and co-variance terms, while the turbulent combustion models close the combustion source term in these equations.

We consider the Smagorinsky models as the baseline LES turbulence model. We observe that the eddy viscosity and gradient diffusion assumptions that lie at the heart of these methods face significant challenges in their ability to capture back-scatter that is significant for non-reacting turbulent flows and, possibly, even more important for reacting turbulent flows. In this regard, we remark that the velocity-composition transported-PDF methods offer an alternate approach to close these terms and may represent a valuable means to evaluate such physical phenomena. The major shortcoming of the hybrid RANS/LES models or DES models lies in the lack of consistency in the definition of the statistical quantities in the two forms of the equations. In the RANS case, they represent the entire energy content of the turbulent field, while in the LES regions, they represent the energy content in the sub-grid or unresolved scales. Appropriate methods for transitioning these terms must be devised in the intermediate regions between RANS and LES regions.

A variety of turbulent combustion models are considered. All of them fall short in their ability to properly capture compressible phenomena, in part because the overwhelming amount of their development has focused on low Mach combustion. Of the models considered, flamelets are to be viewed more as a combustion model rather than a turbulent combustion model. The extension to turbulent combustion is typically achieved through an assumed PDF which is not competitive with more physics-based distribution functions. Even in the area of combustion modeling, there are significant limitations to the generality of the flamelet tables. A fundamental issue is the assumption of a thin flame, which is clearly violated in the case of distributed-reaction problems at low-Da numbers. Likewise, the use of a laminar flow field solution to construct the tables means that fundamental non-equilibrium phenomena related to turbulence interactions are not represented in the tables. Perhaps, more fundamentally, the efficacy of using a small number of reaction progress variables and conserved scalars to represent a large-dimensional manifold remains questionable. The linear eddy model has more general applicability in terms of flame regimes and flow conditions since no fundamental scale-related assumptions are made in their development. In addition, it invokes the low Mach number

assumption only in the sub-grid, and not throughout the entire flowfield. Nevertheless, the absence of diffusion in the large-scale and the arbitrary Lagrangian advective formulation lead to questions about the accuracy of these methods. Finally, the transported-PDF method also promises generality in terms of combustion regimes and flow conditions. However, the development of the method for compressible flows is still relatively new. It seems to us that the construction of compressible transported-PDF methods for the closure of the stress and source terms in the system of conservation laws would be a promising approach towards gaining confidence in their ability to model these terms.

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References

[1]U. Piomelli, Large-eddy simulation: achievements and challenges. *Progress in Aerospace Sciences*, 35:635–362, 1999.

[2]P. R. Spalart. Detached-eddy simulation. *Annual Review of Fluid Mechanics*, 41:181–202, 2009.

[3]N. Peters. *Turbulent Combustion.* Cambridge Monographs on Mechanics, 2000.

[4]A.R.Kerstein. Linear-Eddy Model of Turbulent Transport. *Combustion and Flame*, 75:397–413, 1989.

[5]S. Menon and A.R.Kerstein. Stochastic Simulation of the Structure and Propagation Rate of Turbulent Premixed Flames. *Proceedings of the Combustion Institute*, 24:443–450, 1992.

[6]S. B. Pope, PDF Methods for Turbulent Reactive Flows. *Progress in Energy and Combustion Sciences*, 11:119–192, 1985.

[7]S. Sardeshmukh, Comprehensive Computational Modeling of Hypergolic Propellant Ignition, Purdue University, 2013.

[8]M. Harvazinski, Modeling Self-Excited Combustion Instabilities Using A Combination Of Two- And Three-Dimensional Simulations, Purdue University, 2012.

[9]U.Piomelli, W. H. Cabot, P. Moin, and S. Lee, Subgridscale backscatter in turbulent and transitional flows. *Physics of Fluids A*, 3:1766, 1991.

[10]C. Menneveau and J. Katz. Scale-invariance and turbulence models for large-eddy simulation. *Annual Review of Fluid Mechanics*, 32:1–32, 2000.

[11]Poinsot T, Veynante D. Theoretical and numerical combustion. second ed., Philadelphia, PA: R.T. Edwards Inc., 2005.

[12]J. C. Oefelein, Large eddy simulation of turbulent combustion processes in propulsion and power systems. *Progress in Aerospace Sciences*, 42:2–37, 2006.

[13]A. Leonard. Energy cascade in large eddy simulation of turbulent fluid flow. *Adv. Geophys.*, 18A:237-248, 1974.

[14]J. Smagorinsky, General circulation experiments with the primitive equations. I. The basic experiment. *Mon Weather Rev*, 91:99-164, 1963.

[15]M. Germano, U. Piomelli, P. Moin, and W. Cabot. A dynamic subgrid-scale eddy viscosity model. *Phys. Fluids A-Fluid*, 3:1760–1765, 1991.

[16]D.K. Lilly. A proposed modification of the Germano subgrid scale closure method. *Phys. Fluids A*, 4:633–635, 1992.

[17]S.B.Pope, *Turbulent Flows*, Cambridge University Press, 2000.

[18]P.A. Cocks, V. Sankaran and M. Soteriou, Is LES of reacting flows predictive? Part 1: Impact of numerics, AIAA Paper 2013-0170, 51st AIAA Aerospace Sciences Meeting, Texas, 2013.

[19]Schumann, U., Subgrid Scale Model for Finite Difference Simulations of Turbulent Flows in Plane Channels and Annuli, *Journal of Computational Physics*, Vol. 18, Aug. 1975, pp. 376404.

[20]S. Menon and N. Patel. Subgrid Modeling for Simulation of Spray Combustion in Large-Scale Combustors. *AIAA Journal*, 44(4):709–723, 2006.

[21]M. Strelets. Detached Eddy Simulation of Massively Separated Flows. *39th AIAA Aerospace Sciences Meeting and Exhibit*, 2001.

[22]H. Xiao and P. Jenny. A consistent dual-mesh framework for hybrid LES/RANS modeling. *Journal of Computational Physics*, 231(4):18481865, 2012.

[23]T. Echekki. *Turbulent Combustion Modeling.* Springer, 2011.

[24]C.D. Pierce. *Progress Variable Approach for Large Eddy Simulation of Turbulent Combustion.* PhD thesis, Stanford University, 2001.

[25]Ihme, M., Cha, C., and Pitsch, H. Prediction of local extinction and re-ignition effects in non-premixed turbulent combustion using a flamelet/progress variable approach. *Proc. of the Combustion Institute*, 30, 2005.

[26]Ihme, M. and See, Y.C. Prediction of autoignition in a lifted methane/air flame using an unsteady/progress variable model. *Combustion and Flame*, 157, 2010.

[27]S.B.Pope, Small scales, many species and the manifold challenges of turbulent combustion. *Proceedings of the Combustion Institute*, 34: 1-31, 2013.

[28]Kerstein, A.R., Ashurst, W.T., Wunsch, S and Nilsen, V., One-dimensional turbulence: vector formulation and application to free shear flows, *J. Fluid Mechanics*, 447 (2001) 85-109.

[29]Schmidt, R.C., Kerstein, A.R. and McDermott, R., ODTLES: A multi-scale model for 3D turbulent flow based on one-dimensional turbulence modeling, *Comput. Methods Appl. Mech. Engrg.*, 199 (2010) 865-880.

[30]Haworth, D.C., Progress in probability density function methods for turbulent reacting flows, *Progress in Energy and Combustion Science*, 36 (2010) 168-259.

[31]S.B. Pope, Self-conditioned fields for large-eddy simulations of turbulent flows, *J. Fluid Mech.* 652 (2010) 139169.

[32]M.R.H. Sheikhi, T.G. Drozda, P. Givi, F.A. Jaberi, S.B. Pope, *Proc. Combust. Inst.*, 30 (2005) 549556.

[33]Viswanathan, S., Wang, H., and Pope, S.B., Numerical implementation of mixing and molecular transport in LES/PDF studies of turbulent reacting flows, *J. Comp. Phys.*, 230 (2011) 6916-6957.

[34]R.L. Curl, Dispersed phase mixing I: Theory and effects in simple reactors, *AIChE J.* 9 (2) (1963) 175181.

[35]S. Subramaniam, S.B. Pope, A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees, *Combust. Flame*, 115 (1998) 487514.

[36]R. McDermott, S.B. Pope, A particle formulation for treating differential diffusion in filtered density function methods, *J. Comput. Phys.* 226 (1) (2007) 947993.

[37]P. Jenny, S. B. Pope, M. Muradoglu, and D. A. Caughey, A hybrid algorithm for the joint PDF equation of turbulent reactive flows, *J. Comput. Phys.*, 166, 218 (2001).

[38]Popov, P.P. and Pope, S.B., Implicit and explicit schemes for mass consistency preservation in hybrid particle/finite-volume algorithms for turbulent reactive flows, *J. Comp. Phys.*, 257 (2014) 352-373.

[39]B. J. Delarue and S. B. Pope, Application of pdf methods to compressible turbulent flows, *Phys. Fluids*, 9, (9), September, 1997, 2704-2715.

[40]B. J. Delarue and S. B. Pope, Calculation of subsonic and supersonic turbulent reacting mixing layers using probability density function methods, *Phys. Fluids*, 10 (2), February, 1998,487-498.

[41]S. Sarkar, The pressure-dilatation correlation in compressible flows, *Phys. Fluids* 4, 2674 1992.

[42]O. Zeman, Dilatation dissipation: The concept and application in modeling compressible mixing layers, *Phys. Fluids A*, 2, 178,1990.

[43]O. Zeman, On the decay of compressible isotropic turbulence, *Phys. Fluids. A*, 3, 951, 1991.

[44]Welton, W.C. and Pope, S.B., PDF Model Calculations of Compressible Turbulent Flows Using Smoothed particle Hydrodynamics, *J. Comp. Phys.*, 134 (1997) 150-168.

[45]A. T. Hsu, Y.-L. P. Tsai, and M. S. Raju, Probability density function approach for compressible turbulent reacting flows, *AIAA J.*, 7, 1407, 1994.

[46]ZZ Motheou, E., Nicoud, F. and Poinsot, T. Mixed acoustic-entropy combustion instabilities in gas turbines, *J. Fluid Mechanics*, vol. 749, pp. 542-576. (2014).

[47]WW Garby, R., Selle, L. and Poinsot, T, Large-Eddy simulation of combustion instabilities in a varaiable-length combustor, *C.R. Mecanique*, 341, 220-229, (2013).

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Fundamental Physics and Model Assumptions in Turbulent Combustion Models for Aerospace Propulsion

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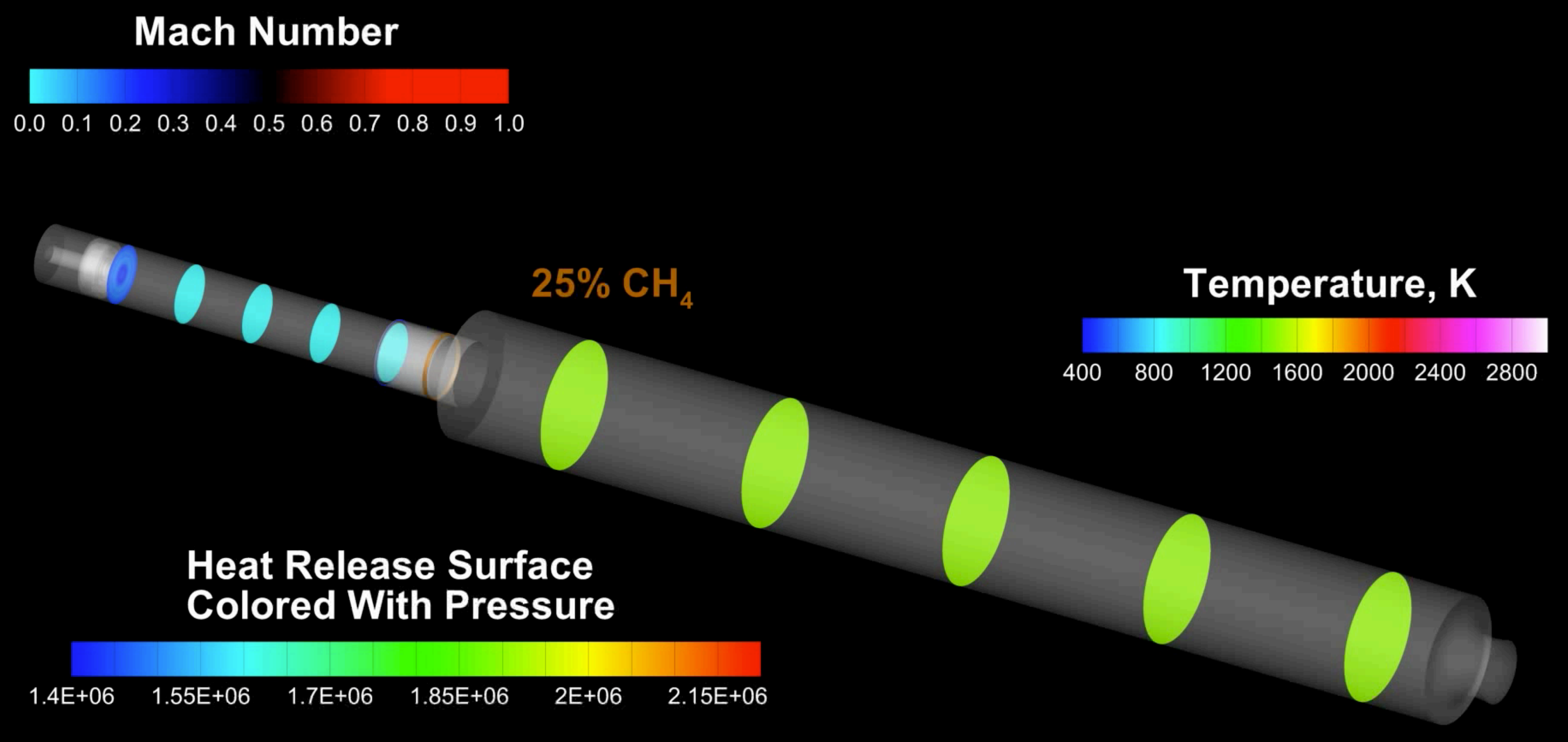
Combustion Stability



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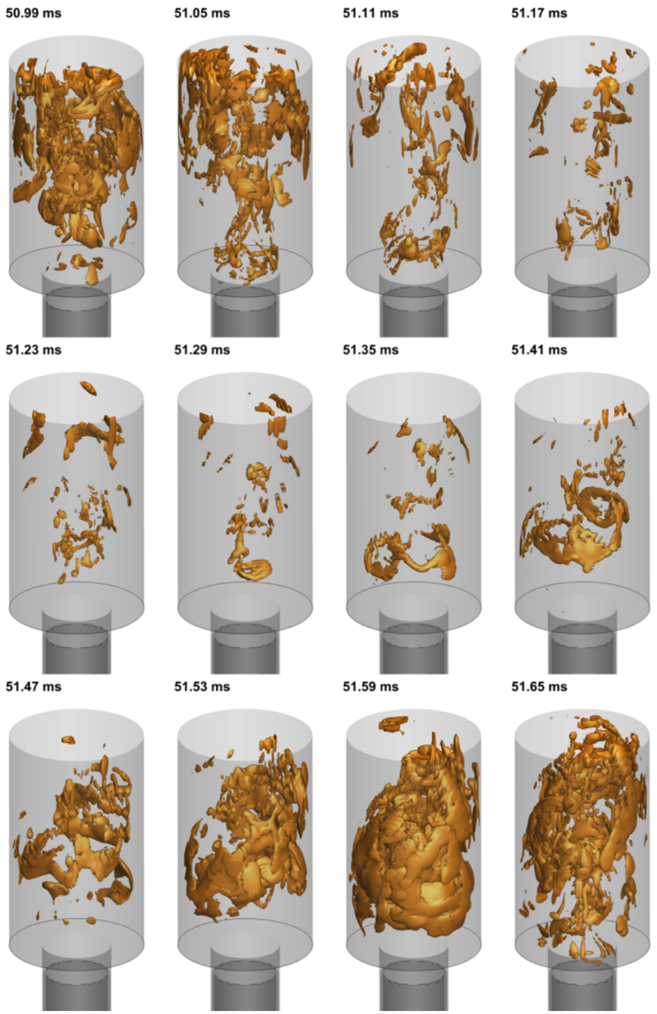
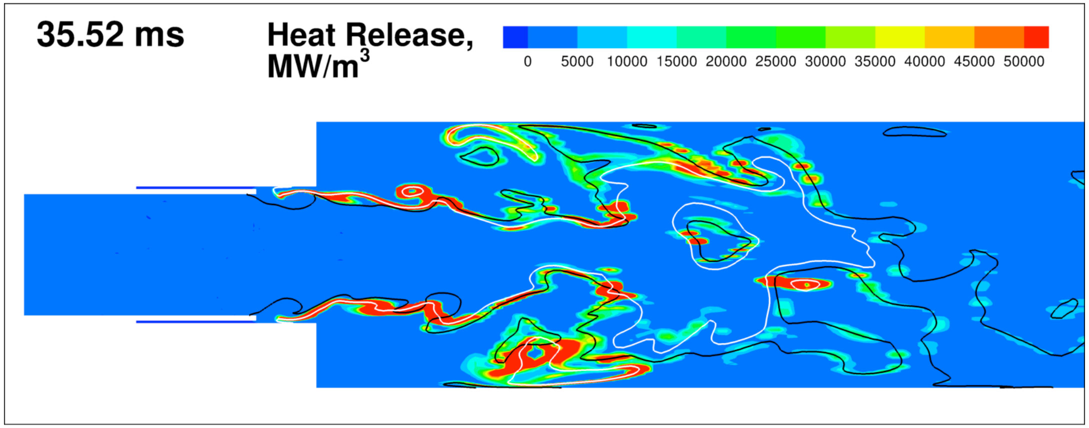
Combustion Dynamics





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Black Line $Z = Z_{st}$

White Line $T = 2000$ K

Goals

- **Model assumptions for Air Force relevant conditions**
  - Rockets, gas turbines, augmentors, scramjets
- **Key Physical Phenomena**
  - High-speeds
  - High pressures
  - Compressible physics - shocks, dilatation, baroclinic
  - Acoustics-combustion-turbulence interactions
- **Validation criteria for reacting-LES**
  - Turbulence effects on chemistry
  - Chemistry effects on turbulence

Conservation Laws

Continuity:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i) = 0$$

Momentum:

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{u}_i) + \frac{\partial}{\partial x_j}(\overline{\rho}\widetilde{u}_j\widetilde{u}_i) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\overline{\tau}_{ji} - \overline{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j))$$

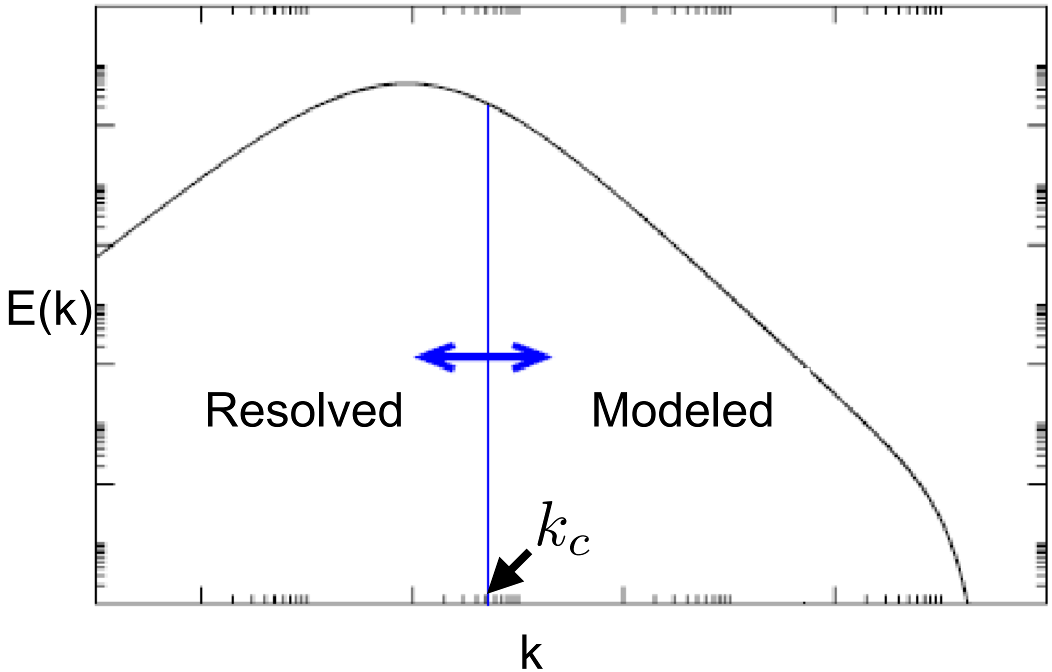
Energy:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{h}_0\right) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{h}_0\right) = \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{u_i\tau_{ij}} - \overline{q}_i - \overline{\rho}(\widetilde{u_j h_0} - \widetilde{u}_j\widetilde{h}_0)\right)$$

Species:

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{Y}_l) + \frac{\partial}{\partial x_j}\left(\overline{\rho}\widetilde{u}_j\widetilde{Y}_l\right) = \frac{\partial}{\partial x_i}(-\overline{\rho}\widetilde{V_{l,i}Y_l}) \boxed{+\overline{\dot{\omega}_l}+} \frac{\partial}{\partial x_j}\left[\overline{\rho}\left(\widetilde{u_j Y_l} - \widetilde{u}_j\widetilde{Y}_l\right)\right]$$

Grid Resolution



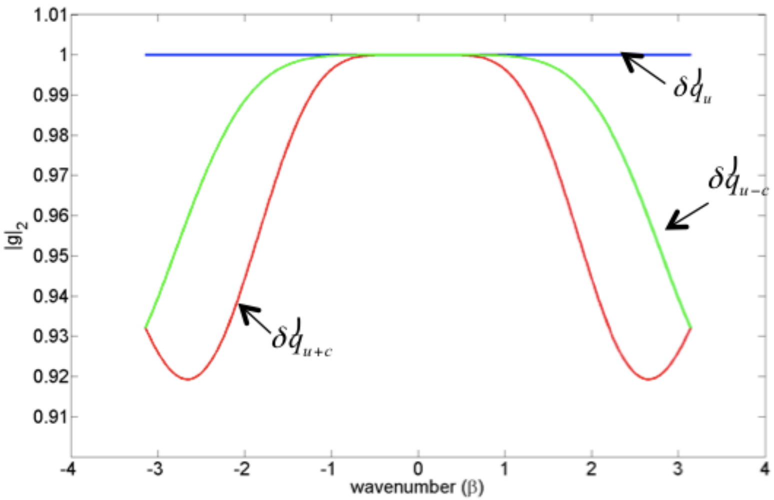
$$\Delta_F = \pi / k_c$$ Usually, grid size: $$\Delta = \Delta_F$$

But, in fact: $$\Delta = \Delta_F / N$$

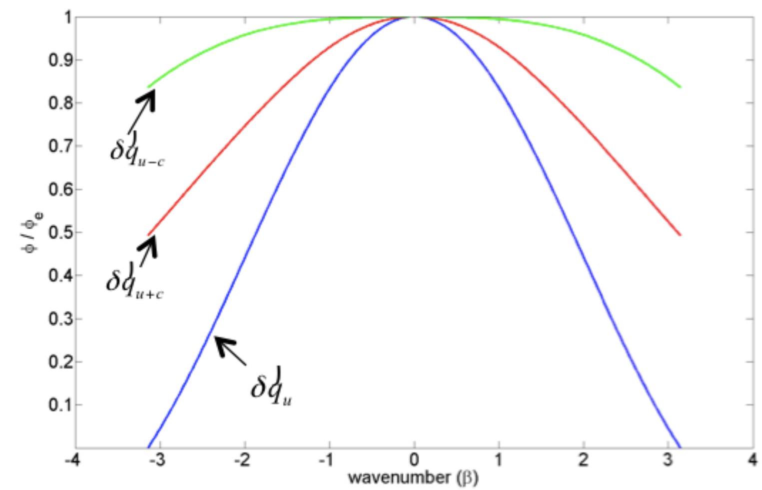
Von Neumann Stability Analysis

Staggered Grid Schemes

Growth



Phase



tol < 1.0% Scheme	Metric	Collocated			Collocated w/ 4th order Artificial Dissipation:			Staggered		
		$\delta \hat{q}_u$	$\delta \hat{q}_{u+c}$	$\delta \hat{q}_{u-c}$	$\delta \hat{q}_u$	$\delta \hat{q}_{u+c}$	$\delta \hat{q}_{u-c}$	$\delta \hat{q}_u$	$\delta \hat{q}_{u+c}$	$\delta \hat{q}_{u-c}$
Crank-Nicolson	**G.F.**	**5**	**5**	**5**	**31**	**29**	**29**	**5**	**5**	**5**
	P.E.	**25**	**29**	**25**	**25**	**29**	**25**	**25**	**23**	**11**
RK4	**G.F.**	**5**	**13**	**7**	**31**	**31**	**31**	**11**	**13**	**11**
	P.E.	**23**	**23**	**23**	**23**	**23**	**23**	**25**	**17**	**11**

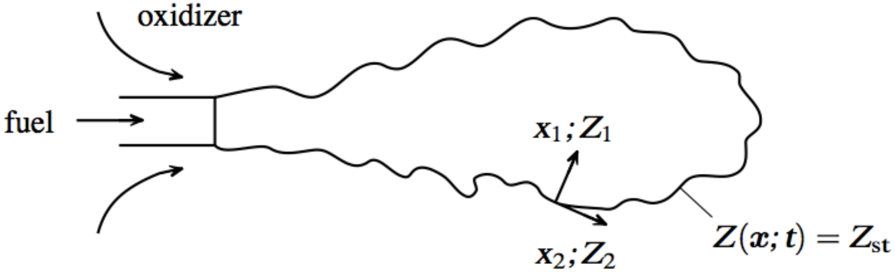
Other Challenges

- **Implicit vs. explicit filtering**
- **Effects of numerical dissipation on sub-grid model**
  – Validity of SGS model definition
- **Ability to capture back-scatter**
  – Combustion adds energy in the smallest scales
- **Gradient diffusion models for scalar transport♀**
  – Validity for reacting turbulence
- **Near-wall LES treatment♀**
- **Hybrid RANS/LES♀**
  – Consistency of TKE defn in RANS and LES regions

♀ - Collaboration with Ez Hassan/RQH

Flamelet Model

- **Basic Assumptions**
  - Pressure assumed to be constant, i.e., low Mach
  - Velocity field is specified from a canonical (but unrelated) problem
  - Assumption of equal diffusion coefficients
  - Presumed PDF model



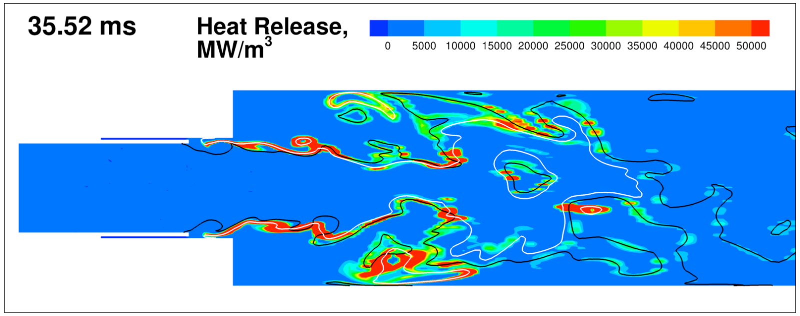
Turbulent Combustion, N. Peters.

$$\boxed{\frac{\rho}{2}\chi\frac{\partial^2 \psi_i}{\partial Z^2} + \dot{w}_i = 0}$$

Flamelet Equation

Comments

- **Other Assumptions**
  - Flame location at stoichiometric line
  - Inconsistency between premixed and non-premixed formulations
  - Neglects thermal effects of neighboring flamelets or walls
  - Unsteady effects are represented qualitatively



Harvazinski et al., 2013

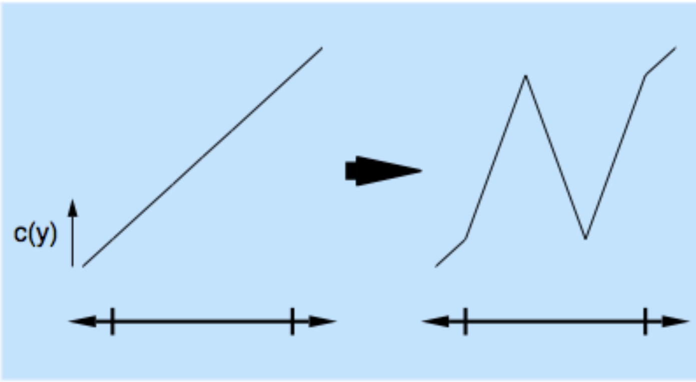
Point-of-View

- **Conservation Laws**
  - Continuity, mom, energy, species
  - Conventional LES closures for stress terms
  - Still need closure of the combustion source term
- **Flamelet Equations**
  - Reactive scalars - energy, species mass fractions
  - Use only to close combustion source terms
- **Dual species and temperature solutions**
  - Provide basis for error estimation

Approach provides a clear basis for the evaluation of flamelet assumptions specifically for turbulent combustion closure as opposed to using flamelets for combustion closure as well.

Linear Eddy Model

- **Key Element - Triplet Maps**
  - Inserts a "1D" eddy in sub-grid
    - compresses the original profile in a given length interval (eddy size) into one-third of the length
    - triplicates the profile and reverses middle section for continuity
    - eddy location, size and frequency are determined stochastically
  - Provides effect of 3D eddy along line-of-sight



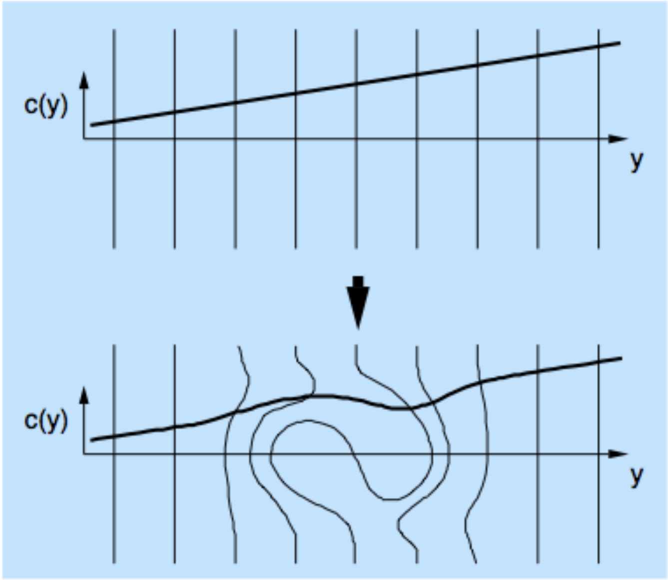


Figure from: Kerstein, 2013.

LEM Solution

Sub-grid Solution:

$$Y_k^{m+1} - Y_k^m = \int_{t_m}^{t_m + \Delta t_{LEM}} -\frac{1}{\rho^m}\left(F_{k,stir} + \frac{\partial}{\partial s}\left(\rho V_k Y_k\right)^m - \dot{w}_k\right) dt$$

Sub-grid stirring **Explicit** **ODE solver**

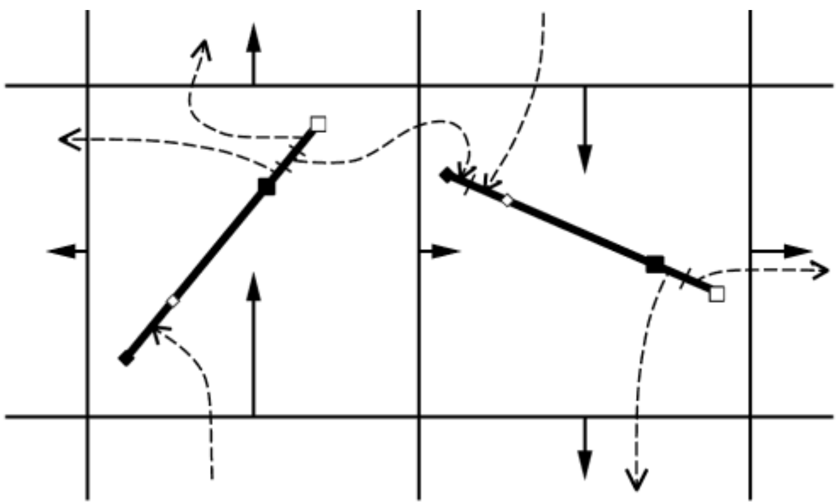


Figure from: Echeki, 2010.

Large scale advection step done by Lagrangian splicing.

Comments

- **Constant pressure assumption in sub-grid solution**
- **Presence of two temperatures**
  - From the resolved grid energy equation
  - Sub-grid energy equation - approximate form used
- **DNS Limit**
  - Inconsistency due to no inter-LES grid species diffusion
- **Implicit solution of the LEM equations**
  - Large scale advective step stymies implicit method

Approach

- **Conservation laws**
  - Mass, momentum, energy and species equations
  - Reynolds stresses using standard closures
- **LEM**
  - Use 1D LEM sub-grid elements to close combustion
- **Dual species and temperature solutions**
  - Provide basis for error estimation

This approach provides a clear basis for the evaluation of the LEM assumptions for turbulent combustion closure and removes other assumptions from the large-scale resolved scales.

PDF Models

- **PDF-Transport Equation**
  - Joint PDF equation can be written for velocity-composition-turbulent frequency, or for velocity-composition, or just for composition
  - Turbulent combustion closure treated exactly
  - Scalar-mixing must be modeled

PDF Transport Equation

$$\langle\rho\rangle\frac{\partial\tilde{f}}{\partial t}+\langle\rho\rangle V_j\frac{\partial\tilde{f}}{\partial x_j}-\frac{\partial\langle p\rangle}{\partial x_j}\frac{\partial\tilde{f}}{\partial V_j}+\frac{\partial}{\partial\psi_j}(\langle\rho\rangle S_k\tilde{f})=\frac{\partial}{\partial V_j}((\langle-\frac{\partial\tau_{ij}}{\partial x_i}+\frac{\partial p'}{\partial x_j}(V,\psi)\rangle\tilde{f})+\frac{\partial}{\partial\psi_k}((\langle\frac{\partial J_i^{\alpha}}{\partial x_i(V,\psi)}\rangle\tilde{f})$$

All LHS terms are closed

All RHS terms must be modeled

Turbulent Combustion Closure

$$\tilde{S}_k=\int S_k(\psi)\tilde{f}d\psi$$

Comments

- **Low Mach assumption commonly applied**
  - Compressible version with joint-PDF of velocity-composition-frequency-enthalpy-pressure has been proposed, but not commonly used
- **Scalar Mixing Models**
  - Modeled portion of PDF methods
- **DNS Consistency recently pursued for mixing models**
  - Allows treating differential diffusion correctly
  - Reduces to DNS in limit of vanishing filter width
- **FDF typically used for LES**
  - Recent interpretations involve defining PDF as self-conditioned fields

Approach

- **Conservation laws in resolved scale**
  - LES equations for mass, momentum, energy, species
- **Joint-PDF Transport**
  - Close Reynolds stress terms using joint-PDF
  - Close turbulent combustion sources using joint-PDF
- **Dual species and temperature solutions**
  - Provide formal basis for error estimation

Again, this approach provides a clear basis for the evaluation of PDF assumptions for sub-grid closure and removes all other assumptions from the large-scale resolved scales.

Road to Model Validation

- **Focus on Air Force relevant conditions**
  - High speed, high pressure, compressible, acoustics
- **Use DNS consistency as evaluation framework**
  - Separate sub-grid closure from other model elements
  - Approach is <u>only</u> an evaluation step
- **DNS solutions are key to validation**
  - Need to establish strong numerical basis for DNS
  - Need to go to smallest scales - maybe even chemistry
  - Control turbulent & chemistry scales to afford DNS
- **Detailed experimental diagnostics are now possible**
  - Need to resolve down to the smallest scales

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